Macromolecular Crystallography

Breakout Session

Larry Shapiro, Lonny Berman, Vivian Stojanoff

15 March 2004

Outline of the Session

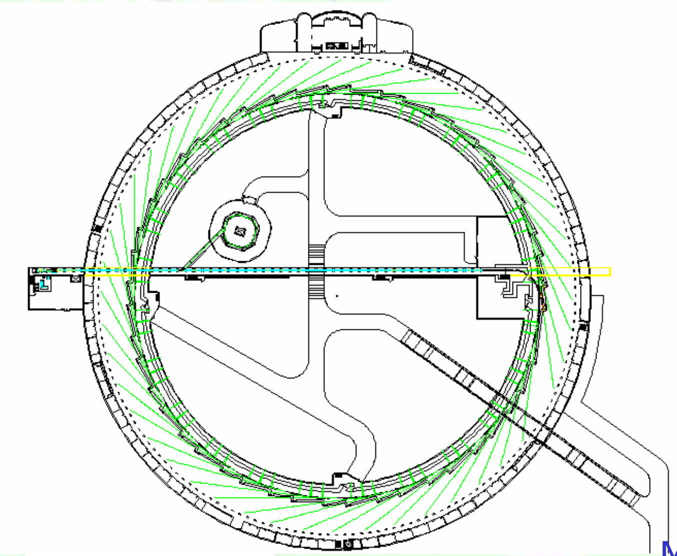
Session Chair: Larry Shapiro

Wayne Hendrickson "Challenges in Biological Crystallography"
Paula Fitzgerald "Practical Experiences in Running a Shared Ownership Beam line"
Elizabeth Duke "Macromolecular Crystallography and Diamond – Exciting Prospects with a Third Generation Source"

Panel Discussion Moderator: LeemorJoshua-Tor

Wayne Hendrickson, Paula Fitzgerald, Elizabeth Duke, Chris Lima, Larry Shapiro and Lonny Berman

Storage Ring Layout



Building Areas	Area [SF] First Flr	Second	Total
Office Block	11,055	8,945	20,000
Utility Corridor	14,578		14,578
Accelerator Tunnel	51,563		51,563
Experimental Floor	111,230		111,230
Office/Lab	64,173	64,173	128,346
Linac Vault - Kly Gallery	12,493	6,068	18,561
			344,278

Medium Energy Storage Ring

- 3 GeV, 24 Fold TBA
- ~ 10^{21} photons/sec/0.1%bw/mm²/mrad²
- ~ 10^{16} photons/sec/0.1%bw
- pulse length 11 psec (13x less then NSLS)
- Flux and Brightness stable to <1%

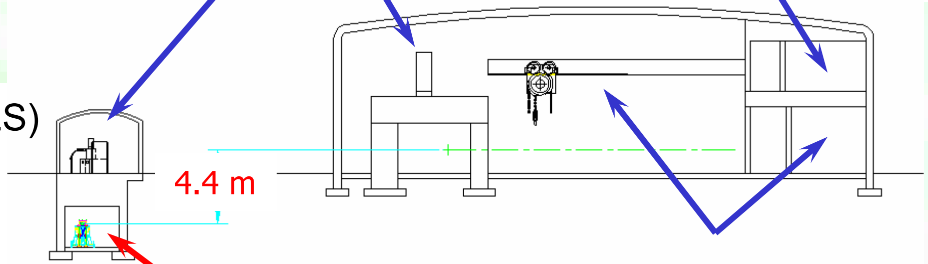
Full Energy Injection

- Linac in this model

Labs and Offices Near Beam lines

Most electrical equipment directly over machine it services

Offices & Common Areas



Crane coverage over limited Assembly Area

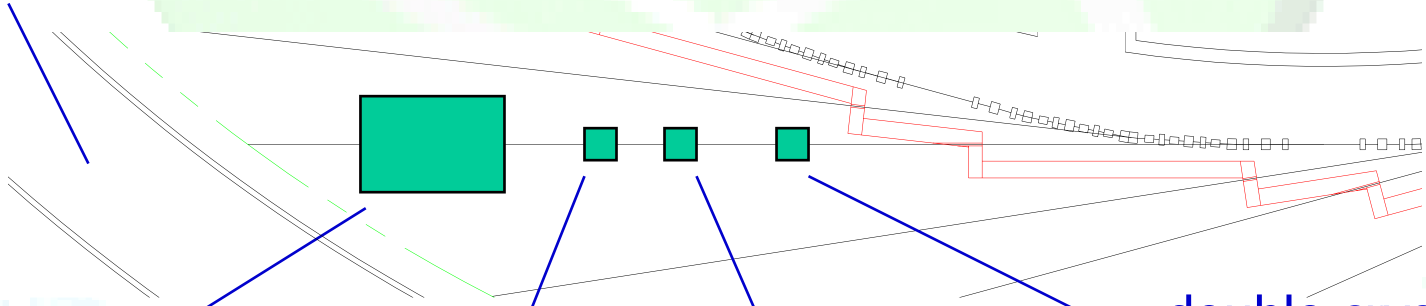
Labs & Common Areas

Linac Below grade to use earth shielding

Proposed Bio-Molecular Crystallography Beam Lines

Operating Energy range: ~3 – 30 KeV
Superconducting Undulators: U14 (5 m long and 14 mm period)
Grazing incidence angle: 3mrad
Si (111) double crystal monochromator
Kirk-Baez mirrors: vertical demagnification 6 (2.5) : 1
horizontal demagnification 7.75(2.8) : 1

space for labs and offices



experimental hutch

vertical focusing mirror

horizontal focusing mirror

double crystal monochromator

Suggested Modes of Operation

- ★ Challenging scientific questions, Virus, Membranes, Molecular Machines > User Access
- ★ Structural "-omics"
- ★ Drug-Development

High-throughput, Automation, Mail-in Service

Performances of NSLS, APS, NSLS-II Beam lines

	NSLS X25	NSLS X29	APS UA	NSLS-II U14
Monochromatic Flux @ 12KeV (ph/sec)	**$3x10^{12}$**	**$3x10^{12}$**	**$1.5x10^{13}$**	**$2.4x10^{14}$**
Energy resolution w/ Si(111) (eV)	12	4	1.8	1.8
Horizontal focus size (mm)	0.7	0.25	0.06	0.075
Vertical focus size (mm)	0.2	0.1	0.03	0.028
Monochromatic intensity (ph/sec/mm^2)	**$2x10^{13}$**	**$1.2x10^{14}$**	**$8x10^{15}$**	**$1.2x10^{17}$**
Horizontal divergence at focus (mrad)	1	1	0.35	0.22
Vertical divergence at focus (mrad)	0.15	0.2	0.1	0.07
Time to 1/e crystal “death” (s)	2500	420	6	0.4

Challenges

The high brightness and flux of the proposed machine and the short lifetime of the samples in such conditions pose new technical challenges

Beam line requirements

End station design

Control and Automation

Detectors

Needs of a diverse User Community need to be addressed

To address these requirements

NSLS II beam lines will incorporate fully automated controls. The *goal* is an end – to – end characterization capability. This could be achieved with a two layer system in which the top (artificial intelligence) layer reasons symbolically with the monitoring and diagnostic sensors and the bottom layer (procedural control) translates them in a set of actuator adjustments

Currently under development:

automated sample changer

artificial intelligence pattern recognition

NSLS THE FUTURE
National Synchrotron Light Source

What we would like to hear your thoughts:

- Beam line issues: how many, mixture of ID and BM, optics
- End Stations: mixture of reconfigurable and fix setup stations
  detectors
  automation
  specialized instrumentation (spectroscopy, lasers, pressure cells, magnetic field, etc.)
  specialized support infrastructure (hazard levels, Lab space)
- User issues: support, training
  quality of life (housing, food facilities, transportation, etc)

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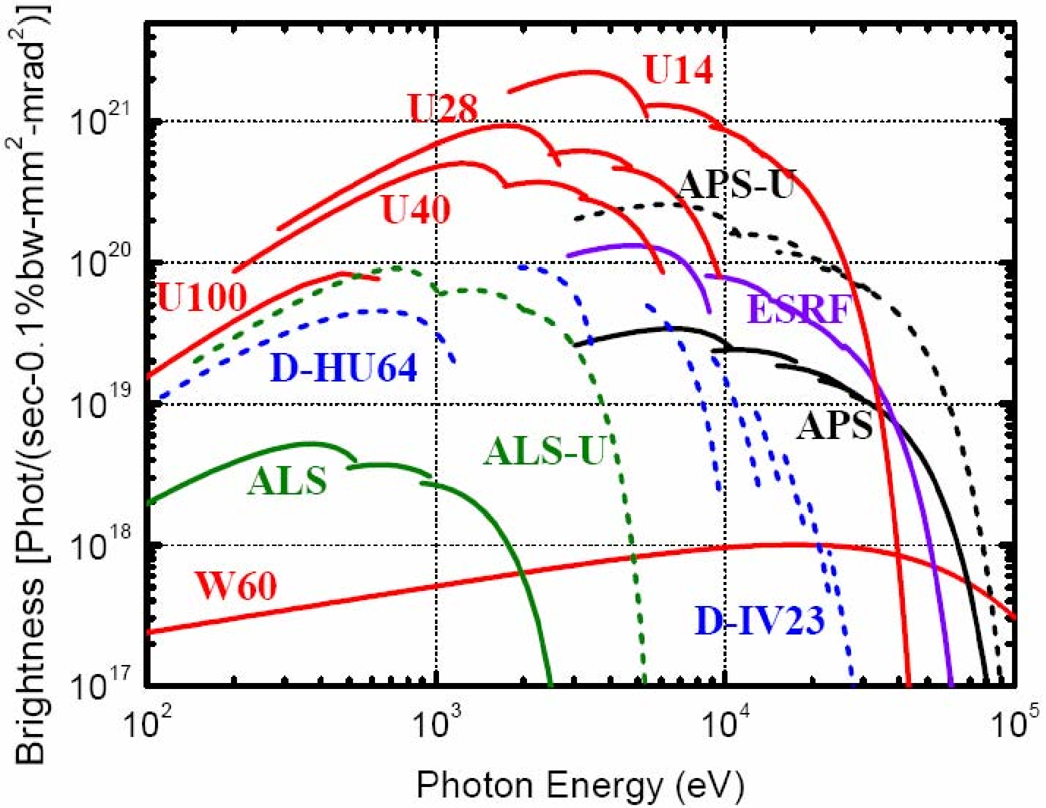
The Machine

	NSLSII	NSLS
Energy (GeV)	3.0	2.8
Current (mA)	500	280
RF Frequency (MHz)	500	52.88
Emittance (ε_x, ε_y) (nm)	1.5, 0.008	78, 0.133
Beam size (σ_x, σ_y) (μm)	83, 4.2	300, 6
Divergence (σ_x, σ_y), (μrad)	18, 1.8	260, 35
Bunch Length (rms) (psec)	11	141
Circumference (m)	620	170.1
Number of Insertion Devices	21	6

The Machine

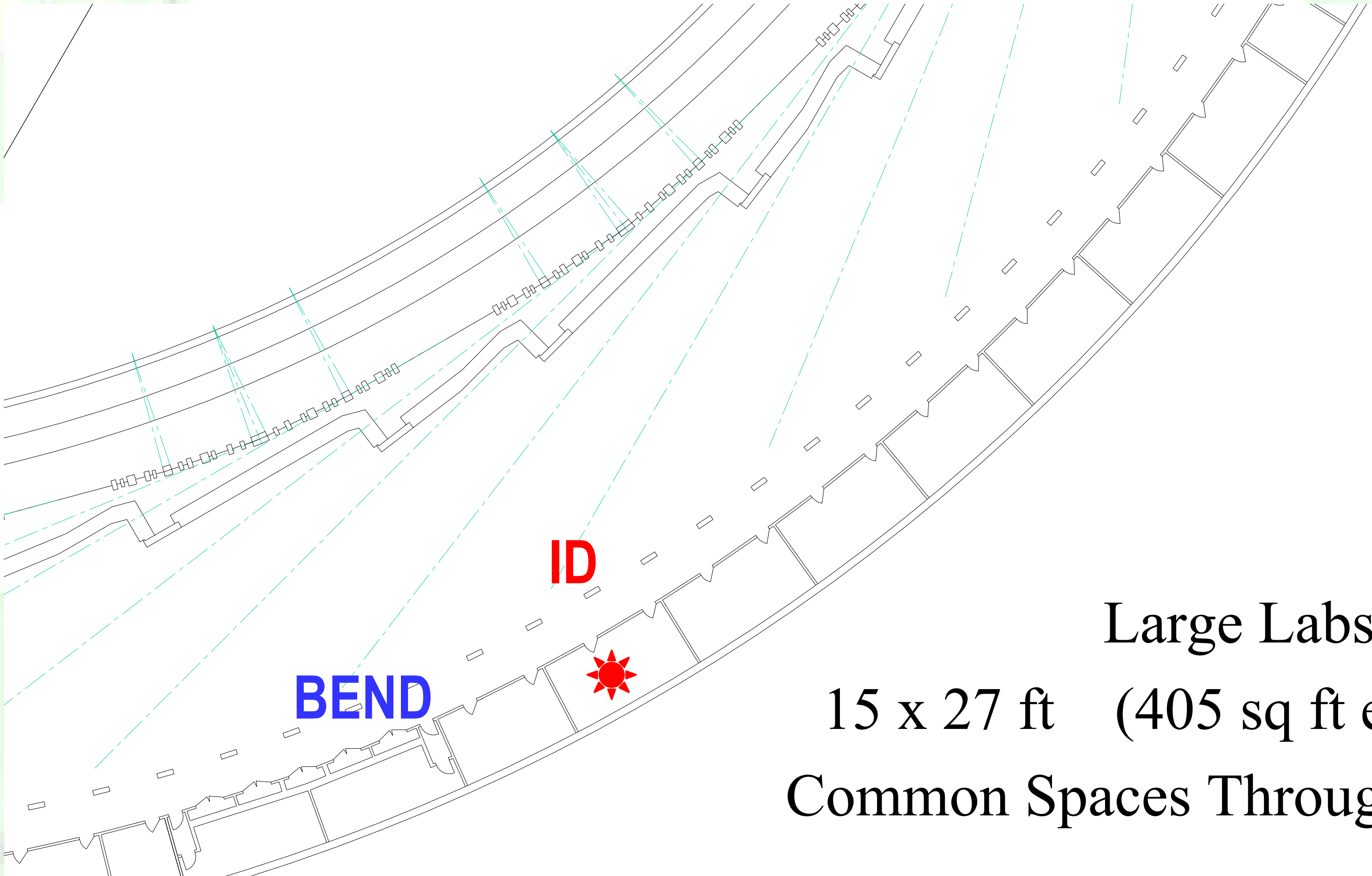
Electron Energy 3.0 GeV
Current 500 mA

Circumference 620 (m)
Number of ID's > 20
Top off operation
Superconducting small gap undulators
Upgrade potential energy recovery linac



THE FUTURE
NATIONAL SYNCHROTRON LIGHT SOURCE
NSLS

Floor Layout



Large Labs (66)

15 x 27 ft   (405 sq ft each)

Common Spaces Throughout

Design concept distributes labs and offices.